Furan

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.88

Global applicability domain: Inside

Local applicability domain index: 5.55e-01

Confidence level: 8.06e-01

Nearest Neighbors from the Training Set

Image not found
Diethyl ether
Measured: 5.37
Predicted: 4.72

Image not found
Furan
Measured: 5.01
Predicted: 4.88

Image not found
Piperidine, 1-methyl-
Measured: 4.47
Predicted: 5.88

Image not found
2-Nitropropane
Measured: 8.32
Predicted: 7.41

Image not found
6-Nitrobenzimidazole
Measured: 2.51
Predicted: 3.81